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1H NMR spectra, dipole moments, and conformations of 3-oxo-6,7-benzo-1,5,3-dioxaphosphepines

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Abstract

1H NMR spectroscopy, measurements of dipole moments, and the Kerr effect have been used to study the conformational structure in solutions of 3-X-3-oxo-6,7-benzo-1,5,3-dioxaphosphepines (X=Me, Et, Ph, Cl, NEt2, OEt, OPh). On the basis of x-ray diffraction data, by means of the Dillen-Geise method, possible conformers of the seven-membered ring have been described quantitatively: chair, twist, and twist-boat. It has been shown that the compounds are characterized by a three-component equilibrium of chair and flexible forms. The relative populations of the conformers depend on the nature of the substituent X. The relationships in internal rotation around the P-Ph and P-O(R) bonds are discussed. © 1991 Plenum Publishing Corporation.

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